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                 Web Page URLs for STN Seminar Schedule - N. America
NEWS
      1
                  "Ask CAS" for self-help around the clock
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      2
                 New pricing for the Save Answers for SciFinder Wizard within
         SEP 01
NEWS
                  STN Express with Discover!
                 KOREAPAT now available on STN
         OCT 28
NEWS
      4
         NOV 30 PHAR reloaded with additional data
      5
 NEWS
 NEWS 6 DEC 01
                 LISA now available on STN
                 12 databases to be removed from STN on December 31, 2004
     7 DEC 09
 NEWS
 NEWS 8 DEC 15
                 MEDLINE update schedule for December 2004
 NEWS 9 DEC 17
                 ELCOM reloaded; updating to resume; current-awareness
                  alerts (SDIs) affected
                 COMPUAB reloaded; updating to resume; current-awareness
      10 DEC 17
NEWS
                  alerts (SDIs) affected
                 SOLIDSTATE reloaded; updating to resume; current-awareness
 NEWS
      11 DEC 17
                  alerts (SDIs) affected
                 CERAB reloaded; updating to resume; current-awareness
      12 DEC 17
 NEWS
                  alerts (SDIs) affected
                 THREE NEW FIELDS ADDED TO IFIPAT/IFIUDB/IFICDB
 NEWS 13 DEC 17
                 EPFULL: New patent full text database to be available on STN
 NEWS 14 DEC 30
                 CAPLUS - PATENT COVERAGE EXPANDED
 NEWS 15 DEC 30
                 No connect-hour charges in EPFULL during January and
      16 JAN 03
 NEWS
                  February 2005
                 CA/CAPLUS - Russian Agency for Patents and Trademarks
 NEWS
      17 FEB 25
                  (ROSPATENT) added to list of core patent offices covered
                 STN Patent Forums to be held in March 2005
 NEWS
     18 FEB 10
                 STN User Update to be held in conjunction with the 229th ACS
      19 FEB 16
                  National Meeting on March 13, 2005
                 PATDPAFULL - New display fields provide for legal status
 NEWS 20 FEB 28
                  data from INPADOC
                 BABS - Current-awareness alerts (SDIs) available
 NEWS 21 FEB 28
                 MEDLINE/LMEDLINE reloaded
 NEWS 22 FEB 28
                 GBFULL: New full-text patent database on STN
NEWS 23 MAR 02
                 REGISTRY/ZREGISTRY - Sequence annotations enhanced
 NEWS 24 MAR 03
                 MEDLINE file segment of TOXCENTER reloaded
 NEWS 25 MAR 03
              JANUARY 10 CURRENT WINDOWS VERSION IS V7.01a, CURRENT
 NEWS EXPRESS
              MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
               AND CURRENT DISCOVER FILE IS DATED 10 JANUARY 2005
               STN Operating Hours Plus Help Desk Availability
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FILE 'HOME' ENTERED AT 16:22:25 ON 15 MAR 2005

=> file reg

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION

0.21

0.21

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 16:22:39 ON 15 MAR 2005 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2005 American Chemical Society (ACS)

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STRUCTURE FILE UPDATES: 14 MAR 2005 HIGHEST RN 845540-96-7 DICTIONARY FILE UPDATES: 14 MAR 2005 HIGHEST RN 845540-96-7

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

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Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\107179581.str

L1 STRUCTURE UPLOADED

=> s 11 SAMPLE SEARCH INITIATED 16:22:57 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 350 TO ITERATE

100.0% PROCESSED 350 ITERATIONS SEARCH TIME: 00.00.01 8 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 5878 TO 8122 PROJECTED ANSWERS: 8 TO 329

L2 8 SEA SSS SAM L1

=> s l1 ful

FULL SEARCH INITIATED 16:23:05 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 7356 TO ITERATE

100.0% PROCESSED 7356 ITERATIONS

124 ANSWERS

SEARCH TIME: 00.00.01

L3 124 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

FULL ESTIMATED COST

ENTRY 161.33 SESSION 161.54

FILE 'CAPLUS' ENTERED AT 16:23:13 ON 15 MAR 2005 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

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FILE COVERS 1907 - 15 Mar 2005 VOL 142 ISS 12 FILE LAST UPDATED: 14 Mar 2005 (20050314/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13

L4

19 L3

=> s 14 and (process or making or make or made or prepar? or synthes?)

2060830 PROCESS

1374299 PROCESSES

3065131 PROCESS

(PROCESS OR PROCESSES)

244396 MAKING

30 MAKINGS

244420 MAKING

(MAKING OR MAKINGS)

205723 MAKE

158981 MAKES

354430 MAKE

(MAKE OR MAKES)

1138680 MADE

23 MADES

1138700 MADE

(MADE OR MADES)

1534101 PREPAR?

115055 PREP

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2025 PREPS
        116881 PREP
                 (PREP OR PREPS)
       1918786 PREPD
            21 PREPDS
       1918801 PREPD
                 (PREPD OR PREPDS)
        106004 PREPG
            12 PREPGS
        106015 PREPG
                 (PREPG OR PREPGS)
       2557303 PREPN
        198667 PREPNS
       2707792 PREPN
                 (PREPN OR PREPNS)
       4488110 PREPAR?
                 (PREPAR? OR PREP OR PREPD OR PREPG OR PREPN)
       1433499 SYNTHES?
             9 L4 AND (PROCESS OR MAKING OR MAKE OR MADE OR PREPAR? OR SYNTHES?
L5
=> d 15 ibib hitstr abs 1-9
    ANSWER 1 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN
                         2004:567636 CAPLUS
ACCESSION NUMBER:
DOCUMENT NUMBER:
                         141:290174
TITLE:
                         Structural Bioinformatics and QSAR Analysis Applied to
                         the Acetylcholinesterase and Bispyridinium Aldoximes
                         Mager, Peter; Weber, Anje
AUTHOR (S):
                         Research Group of Pharmacochemistry, Institute of
CORPORATE SOURCE:
                         Pharmacology and Toxicology, Univ. Leipzig, Saxony,
                         Germany
                         Drug Design and Discovery (2003), 18(4), 127-150
SOURCE:
                         CODEN: DDDIEV; ISSN: 1055-9612
                         Taylor & Francis, Inc.
PUBLISHER:
DOCUMENT TYPE:
                         Journal
                         English
LANGUAGE:
     84871-04-5
TT
    RL: BSU (Biological study, unclassified); PRP (Properties); BIOL
     (Biological study)
        (OSAR anal. applied to acetylcholinesterase and bispyridinium aldoximes
        for qual. structural requirements for reactivating activity against
        organophosphorus agents)
     84871-04-5 CAPLUS
RN
    Pyridinium, 3-(dimethylamino)-1-[[[4-[(hydroxyimino)methyl]pyridinio]metho
CN
    xy]methyl] - (9CI) (CA INDEX NAME)
/ Structure 1 in file .gra /
    The methods of bioinformatics, mol. modeling, and quant.
AB
     structure-activity relationships (QSARs) using regression and artificial
    neural network (ANN) analyses were applied to develop safer aldoxime
     antidotes against poisoning by organophosphorus (OP) agents with high,
    mean, and low aging rates. We start here from a mol. modeling of the
    mouse AChE at an atomistic level. Aim is to predict qual. the structural
     requirements of an aldoxime that shows an unique reactivating activity
     against the three classes of OPs. An antidotal action should occur by a
```

three-site mechanism: the aldoxime groups of the first pyridinium ring should point towards the catalytic site, and the second pyridinium ring

CN

RN

CN

RN

CN

RN

CN

571205-45-3 CAPLUS

INDEX NAME)

```
and its substituents should be anchored at the peripherical and anionic
     subsites. Based on this model, it is predicted that a suitable
     substituent is based on an arginine-like moiety. Then, an ANN-based QSAR
     anal. using a training set of aldoximes with known structure and
     activities was applied. Its input layer consisted of seven nodes: the
    group-membership descriptors that parameterize the type of the OP, the
    logarithms of the distribution coeffs. at pH 7.4 and their squared term,
     the LUMO energies, the scaled molar refractions of the substituents, and
     their squared term. It was shown that the qual. prediction made
    by mol. modeling can be quantified by an ANN prediction.
                               THERE ARE 70 CITED REFERENCES AVAILABLE FOR THIS
REFERENCE COUNT:
                         70
                               RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
    ANSWER 2 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN
                         2004:258121 CAPLUS
ACCESSION NUMBER:
DOCUMENT NUMBER:
                         140:425258
                         Synthesis and Aqueous Ozonation of Some
TITLE:
                         Pyridinium Salts with Alkoxymethyl and Alkylthiomethyl
                         Hydrophobic Groups
                         Pernak, Juliusz; Branicka, Monika
AUTHOR (S):
                         Institute of Chemical Technology and Engineering,
CORPORATE SOURCE:
                         Poznan University of Technology, Poznan, 60-965, Pol.
                         Industrial & Engineering Chemistry Research (2004),
SOURCE:
                         43(9), 1966-1974
                         CODEN: IECRED; ISSN: 0888-5885
                         American Chemical Society
PUBLISHER:
                         Journal
DOCUMENT TYPE:
                         English
LANGUAGE:
    571205-42-0P 571205-43-1P 571205-44-2P
     571205-45-3P 571205-46-4P 571205-47-5P
     571205-48-6P 571205-49-7P 571205-50-0P
     RL: BUU (Biological use, unclassified); PRP (Properties); SPN (Synthetic
     preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
        (preparation and aqueous ozonation of some pyridinium salts with
        alkoxymethyl and alkylthiomethyl hydrophobic groups)
RN 571205-42-0 CAPLUS
     Pyridinium, 3-(dimethylamino)-1-[(heptyloxy)methyl]-, chloride (9CI)
     INDEX NAME)
/ Structure 2 in file .gra /
     571205-43-1 CAPLUS
     Pyridinium, 3-(dimethylamino)-1-[(octyloxy)methyl]-, chloride (9CI)
     INDEX NAME)
/ Structure 3 in file .gra /
     571205-44-2 CAPLUS
     Pyridinium, 3-(dimethylamino)-1-[(nonyloxy)methyl]-, chloride (9CI)
     INDEX NAME)
/ Structure 4 in file .gra /
```

Pyridinium, 1-[(decyloxy)methyl]-3-(dimethylamino)-, chloride (9CI)

```
/ Structure 5 in file .gra /
     571205-46-4 CAPLUS
RN
     Pyridinium, 3-(dimethylamino)-1-[(undecyloxy)methyl]-, chloride (9CI)
CN
     INDEX NAME)
/ Structure 6 in file .gra /
RN
     571205-47-5 CAPLUS
     Pyridinium, 3-(dimethylamino)-1-[(dodecyloxy)methyl]-, chloride (9CI)
CN
     INDEX NAME)
/ Structure 7 in file .gra /
     571205-48-6 CAPLUS
RN
     Pyridinium, 3-(dimethylamino)-1-[(tetradecyloxy)methyl]-, chloride (9CI)
CN
     (CA INDEX NAME)
/ Structure 8 in file .gra /
     571205-49-7 CAPLUS
RN
     Pyridinium, 3-(dimethylamino)-1-[(hexadecyloxy)methyl]-, chloride (9CI)
CN
     (CA INDEX NAME)
/ Structure 9 in file .gra /
     571205-50-0 CAPLUS
RN
     Pyridinium, 3-(dimethylamino)-1-[(octadecyloxy)methyl]-, chloride (9CI)
CN
     (CA INDEX NAME)
/ Structure 10 in file .gra /
     The reaction of ozone with a number of pyridinium salts containing
1-alkoxymethyl
     and 1-alkylthiomethyl substituents was determined at a total substrate
     of 2 q/L. Ozonation of pyridinium salts was strongly dependent on the
     kinds and positions of the substituents in the pyridine ring. The most
     favorable were the third position and the substituents including hydroxyl
     or dimethylamino groups. In an aqueous solution, 1-(alkoxymethyl)-3-
     hydroxypyridinium, 1-(alkylthiomethyl)-3-hydroxypyridinium, and
     1-(alkoxymethyl)-3-(dimethylamino)pyridinium salts reacted with ozone.
     The reaction was fast, and pyridinium salts were quant. removed.
     1-(Alkoxymethyl) - and 1-(alkylthiomethyl)pyridinium chlorides were
     obtained by the Menschutkin reaction. In general, the procedure was
     simple and the reaction was productive and short. During the course of
     this study, we synthesized a new generation of cationic
     surfactants that were extremely reactive with ozone in an aqueous solution
                               THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS
REFERENCE COUNT:
                         31
                               RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
     ANSWER 3 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN
                        2003:346161 CAPLUS
ACCESSION NUMBER:
                         139:149500
DOCUMENT NUMBER:
```

```
The properties of 1-alkoxymethyl-3-hydroxypyridinium
TITLE:
                         and 1-alkoxymethyl-3-dimethylaminopyridinium chlorides
                         Pernak, Juliusz; Branicka, Monika
AUTHOR (S):
                         Department of Chemical Technology, Poznan University
CORPORATE SOURCE:
                         of Technology, Poznan, 60-965, Pol.
                         Journal of Surfactants and Detergents (2003), 6(2),
SOURCE:
                         119-123
                         CODEN: JSDEFL; ISSN: 1097-3958
                         AOCS Press
PUBLISHER:
DOCUMENT TYPE:
                         Journal
LANGUAGE:
                         English
                         CASREACT 139:149500
OTHER SOURCE(S):
     571205-38-4P 571205-39-5P 571205-40-8P
     571205-41-9P 571205-42-0P 571205-43-1P
     571205-44-2P 571205-45-3P 571205-46-4P
     571205-47-5P 571205-48-6P 571205-49-7P
     571205-50-0P
     RL: BSU (Biological study, unclassified); SPN (Synthetic preparation);
     BIOL (Biological study); PREP (Preparation)
        (prepns. and antimicrobial activities of 1-alkoxymethyl-3-
        substituted pyridinium chlorides)
     571205-38-4 CAPLUS
RN
     Pyridinium, 3-(dimethylamino)-1-(propoxymethyl)-, chloride (9CI)
                                                                         (CA
CN
     INDEX NAME)
/ Structure 11 in file .gra /
     571205-39-5 CAPLUS
RN
     Pyridinium, 1-(butoxymethyl)-3-(dimethylamino)-, chloride (9CI)
CN
     NAME)
/ Structure 12 in file .gra /
     571205-40-8 CAPLUS
RN
     Pyridinium, 3-(dimethylamino)-1-[(pentyloxy)methyl]-, chloride (9CI)
CN
     INDEX NAME)
/ Structure 13 in file .gra /
     571205-41-9 CAPLUS
RN
     Pyridinium, 3-(dimethylamino)-1-[(hexyloxy)methyl]-, chloride (9CI)
CN
     INDEX NAME)
/ Structure 14 in file .gra /
     571205-42-0 CAPLUS
RN
     Pyridinium, 3-(dimethylamino)-1-[(heptyloxy)methyl]-, chloride (9CI)
CN
     INDEX NAME)
/ Structure 15 in file .gra /
     571205-43-1 CAPLUS
RN
     Pyridinium, 3-(dimethylamino)-1-[(octyloxy)methyl]-, chloride (9CI)
CN
     INDEX NAME)
```

10/717,958

```
/ Structure 16 in file .gra /
     571205-44-2 CAPLUS
RN
     Pyridinium, 3-(dimethylamino)-1-[(nonyloxy)methyl]-, chloride (9CI)
CN
     INDEX NAME)
/ Structure 17 in file .gra /
RN
     571205-45-3 CAPLUS
     Pyridinium, 1-[(decyloxy)methyl]-3-(dimethylamino)-, chloride (9CI) (CA
CN
     INDEX NAME)
/ Structure 18 in file .gra /
     571205-46-4 CAPLUS
RN
     Pyridinium, 3-(dimethylamino)-1-[(undecyloxy)methyl]-, chloride (9CI)
CN
/ Structure 19 in file .gra /
RN
     571205-47-5 CAPLUS
     Pyridinium, 3-(dimethylamino)-1-[(dodecyloxy)methyl]-, chloride (9CI)
CN
     INDEX NAME)
/ Structure 20 in file .gra /
     571205-48-6 CAPLUS
RN
     Pyridinium, 3-(dimethylamino)-1-[(tetradecyloxy)methyl]-, chloride (9CI)
CN
     (CA INDEX NAME)
/ Structure 21 in file .gra /
RN
     571205-49-7 CAPLUS
     Pyridinium, 3-(dimethylamino)-1-[(hexadecyloxy)methyl]-, chloride (9CI)
CN
    (CA INDEX NAME)
/ Structure 22 in file .gra /
     571205-50-0 CAPLUS
RN
     Pyridinium, 3-(dimethylamino)-1-[(octadecyloxy)methyl]-, chloride (9CI)
     (CA INDEX NAME)
/ Structure 23 in file .gra /
     Several 1-alkoxymethyl-3-substituted-pyridinium chlorides with alkoxy
    chains including from 3 to 18 carbon atoms were prepared by the
     reaction of 3-substituted-pyridine with chloromethyl alkyl ethers. The
     prepared chlorides were examined for their antielectrostatic effects
     and their antimicrobial activities. 1-Dodecyloxymethyl-3-
     dimethylaminopyridinium chloride (23) exhibited strong antimicrobial
     activity and a wide antimicrobial spectrum, similar to the activity of
     benzalkonium chloride. 1-Alkoxymethyl-3-hydroxypyridinium chlorides
```

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activity. The antielectrostatic effect and antimicrobial activities are
     strongly dependent on the kind of substituent at the 3-position in the
    pyridine ring and are greatly affected by an alkoxy chain. Dimethylamino
     group in position three must be present for a high antielectrostatic and
     antimicrobial activity of the agent.
                               THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS
                         20
REFERENCE COUNT:
                               RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
    ANSWER 4 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN
                         2002:325907 CAPLUS
ACCESSION NUMBER:
                         137:201262
DOCUMENT NUMBER:
                         Synthesis and antimicrobial activities of
TITLE:
                         new pyridinium and benzimidazolium chlorides
                         Pernak, Juliusz; Rogoza, Jarostaw; Mirska, Ilona
AUTHOR(S):
                         Poznan University of Technology, Poznan, 60-965, Pol.
CORPORATE SOURCE:
                         European Journal of Medicinal Chemistry (2001), 36(4),
SOURCE:
                         313-320
                         CODEN: EJMCA5; ISSN: 0223-5234
                         Editions Scientifiques et Medicales Elsevier
PUBLISHER:
DOCUMENT TYPE:
                         Journal
LANGUAGE:
                         English
                         CASREACT 137:201262
OTHER SOURCE(S):
    404965-60-2P 452281-20-8P 452281-21-9P
     452281-22-0P
    RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic
    preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant
        (synthesis and antibacterial and antifungal activities of new
        pyridinium and benzimidazolium chlorides)
     404965-60-2 CAPLUS
RN
     Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(undecyloxy)methyl]-,
CN
     chloride (9CI) (CA INDEX NAME)
/ Structure 24 in file .gra /
     452281-20-8 CAPLUS
RN
     Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(nonyloxy)methyl]-,
CN
     chloride (9CI) (CA INDEX NAME)
/ Structure 25 in file .gra /
     452281-21-9 CAPLUS
RN
     Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(decyloxy)methyl]-,
CN
     chloride (9CI) (CA INDEX NAME)
/ Structure 26 in file .gra /
RN
     452281-22-0 CAPLUS
     Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(dodecyloxy)methyl]-,
CN
     chloride (9CI) (CA INDEX NAME)
/ Structure 27 in file .gra /
     404965-58-8P 404965-59-9P 404965-71-5P
```

possess antielectrostatic properties, but are lacking antimicrobial

404965-72-6P 404965-84-0P 404965-85-1P

```
10/717,958
     404965-86-2P 404965-87-3P 404965-88-4P
     404965-89-5P 404965-90-8P 404965-91-9P
     404965-92-0P 404965-93-1P 452281-16-2P
     452281-17-3P 452281-18-4P 452281-19-5P
     452281-23-1P 452281-24-2P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL
     (Biological study); PREP (Preparation)
         (synthesis and antibacterial and antifungal activities of new
        pyridinium and benzimidazolium chlorides)
RN
     404965-58-8 CAPLUS
     Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-(propoxymethyl)-,
CN
     chloride (9CI) (CA INDEX NAME)
/ Structure 28 in file .gra /
     404965-59-9 CAPLUS
RN
     Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(octyloxy)methyl]-,
CN
     chloride (9CI) (CA INDEX NAME)
// Structure 29 in file .gra /
RN
     404965-71-5 CAPLUS
     Pyridinium, 3,3'-(methylenediimino)bis[1-[(nonyloxy)methyl]-, dichloride
CN
     (9CI) (CA INDEX NAME)
/ Structure 30 in file .gra /
     404965-72-6 CAPLUS
RN
     Pyridinium, 3,3'-(methylenediimino)bis[1-(undecyloxy)methyl]-, dichloride
CN
     (9CI) (CA INDEX NAME)
/ Structure 31 in file .gra /
     404965-84-0 CAPLUS
RN
     Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-(propoxymethyl)-,
CN
     chloride (9CI) (CA INDEX NAME)
/ Structure 32 in file .gra /
     404965-85-1 CAPLUS
RN
     Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-(butoxymethyl)-,
CN
     chloride (9CI) (CA INDEX NAME)
/ Structure 33 in file .gra /
RN
     404965-86-2 CAPLUS
     Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-[(pentyloxy)methyl]-,
CN
     chloride (9CI) (CA INDEX NAME)
/ Structure 34 in file .gra /
```

Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-[(hexyloxy)methyl]-,

404965-87-3 CAPLUS

RN

CN

```
10/717,958
    chloride (9CI) (CA INDEX NAME)
/ Structure 35 in file .gra /
RN
     404965-88-4 CAPLUS
    Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-[(heptyloxy)methyl]-,
CN
    chloride (9CI) (CA INDEX NAME)
/ Structure 36 in file .gra /
     404965-89-5 CAPLUS
    Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-[(octyloxy)methyl]-,
CN
     chloride (9CI) (CA INDEX NAME)
/ Structure 37 in file .gra /
    404965-90-8 CAPLUS
RN
CN
    Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-[(nonyloxy)methyl]-,
    chloride (9CI) (CA INDEX NAME)
/ Structure 38 in file .gra /
    404965-91-9 CAPLUS
RN
    Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-[(decyloxy)methyl]-,
CN
    chloride (9CI) (CA INDEX NAME)
/ Structure 39 in file .gra /
RN
    404965-92-0 CAPLUS
    Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-[(undecyloxy)methyl]-,
CN
    chloride (9CI) (CA INDEX NAME)
/ Structure 40 in file .gra /
RN
    404965-93-1 CAPLUS
    Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-[(dodecyloxy)methyl]-,
CN
    chloride (9CI) (CA INDEX NAME)
/ Structure 41 in file .gra /
     452281-16-2 CAPLUS
RN
    Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-(butoxymethyl)-,
CN
     chloride (9CI) (CA INDEX NAME)
/ Structure 42 in file .gra /
RN
     452281-17-3 CAPLUS
     Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(pentyloxy)methyl]-,
CN
     chloride (9CI) (CA INDEX NAME)
/ Structure 43 in file .gra /
```

```
452281-18-4 CAPLUS
RN
     Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(hexyloxy)methyl}-,
CN
     chloride (9CI) (CA INDEX NAME)
/ Structure 44 in file .gra /
RN
     452281-19-5 CAPLUS
     Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(heptyloxy)methyl]-,
CN
     chloride (9CI) (CA INDEX NAME)
/ Structure 45 in file .gra /
     452281-23-1 CAPLUS
RN
     Pyridinium, 3,3'-(methylenediimino)bis[1-[(decyloxy)methyl]-, dichloride
CN
     (9CI) (CA INDEX NAME)
/ Structure 46 in file .gra /
ВN
     452281-24-2 CAPLUS
    Pyridinium, 3,3'-(methylenediimino)bis[1-[(dodecyloxy)methyl]-, dichloride
CN ·
     (9CI) (CA INDEX NAME)
/ Structure 47 in file .gra /
GΙ
/ Structure 48 in file .gra /
    Novel pyridinium, e.g I, and benzimidazolium, e.g. II, chlorides were
AB
     obtained in high yield. The antimicrobial activities of three homologous
     series of pyridinium and benzimidazolium chlorides against cocci, rods,
     fungi and bacillus were measured. The antimicrobial activities of
    N, N'-bis[3-(1-alkoxymethyl)pyridinium chloride]methylenediamines,
     1-undecyloxymethyl-3-(1-benzimidazolmethylamino)pyridinium,
     1-undecyloxymethyl- and 1-dodecyloxymethyl-3-[1(benzotriazol-1-
    yl) methylamino] pyridinium chlorides exhibited strong activity and wide
     antibacterial spectra similar to the activity of benzalkonium chloride.
                               THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS
REFERENCE COUNT:
                         21
                               RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
                   CAPLUS COPYRIGHT 2005 ACS on STN
    ANSWER 5 OF 9
ACCESSION NUMBER:
                         2001:773384 CAPLUS
DOCUMENT NUMBER:
                         136:263127
                         Synthesis of 3-substituted pyridinium salts
TITLE:
                         Pernak, Juliusz; Rogoza, Jaroslaw
AUTHOR (S):
                         Inst. Chem. Technol. Eng., Poznan Univ. Technol.,
CORPORATE SOURCE:
                         Poznan, 60-965, Pol.
                         ARKIVOC [online computer file] (2000), 1(6), 889-904
SOURCE:
                         CODEN: AKVCFI
                         URL: http://www.arkat.org/arkat/journal/Issue6/ms06-
                         0084.pdf
```

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10/717,958
                         ARKAT Foundation
PUBLISHER:
DOCUMENT TYPE:
                         Journal; (online computer file)
                         English
LANGUAGE:
     404965-58-8P 404965-59-9P 404965-60-2P
     404965-61-3P 404965-63-5P 404965-64-6P
     404965-65-7P 404965-66-8P 404965-67-9P
     404965-68-0P 404965-70-4P 404966-06-9P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation of 3-substituted pyridinium salts)
     404965-58-8 CAPLUS
Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-(propoxymethyl)-,
RN
CN
     chloride (9CI) (CA INDEX NAME)
/ Structure 49 in file .gra /
     404965-59-9 CAPLUS
RN
     Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(octyloxy)methyl]-,
CN
     chloride (9CI) (CA INDEX NAME)
/ Structure 50 in file .gra /
RN
     404965-60-2 CAPLUS
     Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(undecyloxy)methyl]-,
CN
     chloride (9CI) (CA INDEX NAME)
/ Structure 51 in file .gra /
     404965-61-3 CAPLUS
RN
     Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-(propoxymethyl)-,
CN
     bromide (9CI) (CA INDEX NAME)
/ Structure 52 in file .gra /
     404965-63-5 CAPLUS
RN
     Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(octyloxy)methyl]-,
CN
     nitrate (9CI) (CA INDEX NAME)
     CM
          1
     CRN 404965-62-4
     CMF C22 H31 N4 O
/ Structure 53 in file .gra /
     CM
     CRN 14797-55-8
     CMF N O3
```

/ Structure 54 in file .gra /

404965-64-6 CAPLUS

RN

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10/717,958
     Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(octyloxy)methyl}-,
CN
     iodide (9CI) (CA INDEX NAME)
/ Structure 55 in file .gra /
     404965-65-7 CAPLUS
    Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(octyloxy)methyl]-,
CN
    tetrafluoroborate(1-) (9CI) (CA INDEX NAME)
    CM
         404965-62-4
     CRN
     CMF C22 H31 N4 O
/ Structure 56 in file .gra /
     CM
         2
     CRN
        14874-70-5
    CMF
         B F4
    CCI
         CCS
/ Structure 57 in file .gra /
    404965-66-8 CAPLUS
RN
     Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(octyloxy)methyl]-,
CN
    hexafluorophosphate(1-) (9CI) (CA INDEX NAME)
     CM
          1
     CRN 404965-62-4
     CMF C22 H31 N4 O
/ Structure 58 in file .gra /
     CM
          2
         16919-18-9
     CRN
     CMF
         F6 P
     CCI CCS
/ Structure 59 in file .gra /
RN
     404965-67-9 CAPLUS
     Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(octyloxy)methyl]-,
CN
    perchlorate (9CI) (CA INDEX NAME)
     CM
          1
     CRN 404965-62-4
         C22 H31 N4 O
     CMF
```

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10/717,958
/ Structure 60 in file .gra /
    CM
         2
     CRN 14797-73-0
     CMF Cl O4
/ Structure 61 in file .gra /
     404965-68-0 CAPLUS
RN
     Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(dodecyloxy)methyl]-,
CN
     iodide (9CI) (CA INDEX NAME)
/ Structure 62 in file .gra /
     404965-70-4 CAPLUS
RN
     Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(dodecyloxy)methyl]-,
CN
    hexafluorophosphate(1-) (9CI) (CA INDEX NAME)
     CM
         1
     CRN 404965-69-1
     CMF C26 H39 N4 O
/ Structure 63 in file .gra /
          2
     CM
     CRN 16919-18-9
     CMF F6 P
     CCI CCS ·
/ Structure 64 in file .gra /
RN
     404966-06-9 CAPLUS
     Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(dodecyloxy)methyl]-,
CN
     perchlorate (9CI) (CA INDEX NAME)
     CM
          1
     CRN 404965-69-1
     CMF C26 H39 N4 O
/ Structure 65 in file .gra /
     CM
     CRN 14797-73-0
     CMF Cl O4
/ Structure 66 in file .gra /
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404965-71-5P 404965-72-6P 404965-74-8P
IT
     404965-75-9P 404965-76-0P 404965-77-1P
     404965-79-3P 404965-80-6P 404965-81-7P
     404965-84-0P 404965-85-1P 404965-86-2P
     404965-87-3P 404965-88-4P 404965-89-5P
     404965-90-8P 404965-91-9P 404965-92-0P
     404965-93-1P 404965-94-2P 404965-96-4P
     404965-98-6P 404965-99-7P 404966-00-3P
     404966-01-4P 404966-02-5P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of 3-substituted pyridinium salts)
     404965-71-5 CAPLUS
Pyridinium, 3,3'-(methylenediimino)bis[1-[(nonyloxy)methyl]-, dichloride
RN
CN
     (9CI) (CA INDEX NAME)
/ Structure 67 in file .gra /
     404965-72-6 CAPLUS Pyridinium, 3,3'-(methylenediimino)bis[1-(undecyloxy)methyl]-, dichloride
RN
CN
     (9CI) (CA INDEX NAME)
/ Structure 68 in file .gra /
     404965-74-8 CAPLUS
RN
     Pyridinium, 3,3'-(methylenediimino)bis[1-[(octyloxy)methyl]-,
CN
     diperchlorate (9CI) (CA INDEX NAME)
     CM
          1
     CRN 404965-73-7
     CMF C29 H50 N4 O2
/ Structure 69 in file .gra /
     CM
     CRN 14797-73-0
     CMF Cl O4
/ Structure 70 in file .gra /
     404965-75-9 CAPLUS
RN
     Pyridinium, 3,3'-(methylenediimino)bis[1-[(octyloxy)methyl]-, dibromate
CN
           (CA INDEX NAME)
     (9CI)
     CM
          1
     CRN 404965-73-7
     CMF C29 H50 N4 O2
/ Structure 71 in file .gra /
```

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10/717,958
     CM
     CRN
         15541-45-4
     CMF Br 03
/ Structure 72 in file .gra /
     404965-76-0 CAPLUS
RN
     Pyridinium, 3,3'-(methylenediimino)bis[1-(octyloxy)methyl]-, diiodide
CN
     (9CI) (CA INDEX NAME)
/ Structure 73 in file .gra /
     404965-77-1 CAPLUS
Pyridinium, 3,3'-(methylenediimino)bis[1-(octyloxy)methyl]-, dibromide
RN
CN
     (9CI) (CA INDEX NAME)
/ Structure 74 in file .gra /
     404965-79-3 CAPLUS
Pyridinium, 3,3'-(methylenediimino)bis[1-[(dodecyloxy)methyl]-,
RN
CN
     bis[hexafluorophosphate(1-)] (9CI) (CA INDEX NAME)
     CM
          1
     CRN 404965-78-2
     CMF C37 H66 N4 O2
/ Structure 75 in file .gra /
     CM
          2
     CRN 16919-18-9
     CMF F6 P
     CCI CCS
/ Structure 76 in file .gra /
     404965-80-6 CAPLUS
RN
     Pyridinium, 3,3'-(methylenediimino)bis[1-[(dodecyloxy)methyl]-,
CN
     bis[(OC-6-11)-hexafluoroantimonate(1-)] (9CI) (CA INDEX NAME)
     CM
          1
     CRN 404965-78-2
     CMF C37 H66 N4 O2
/ Structure 77 in file .gra /
     CM
     CRN 17111-95-4
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10/717,958
    CMF F6 Sb
    CCI CCS
/ Structure 78 in file .gra /
     404965-81-7 CAPLUS
RN
    Pyridinium, 3,3'-(methylenediimino)bis[1-(dodecyloxy)methyl]-, diiodide
CN
     (9CI) (CA INDEX NAME)
/ Structure 79 in file .gra /
    404965-84-0 CAPLUS
RN
    Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-(propoxymethyl)-,
CN
    chloride (9CI) (CA INDEX NAME)
/ Structure 80 in file .gra /
    404965-85-1 CAPLUS
RN
    Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-(butoxymethyl)-,
CN
    chloride (9CI) (CA INDEX NAME)
/ Structure 81 in file .gra /
   404965-86-2 CAPLUS
    Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-[(pentyloxy)methyl]-,
CN
    chloride (9CI) (CA INDEX NAME)
/ Structure 82 in file .gra /
RN
     404965-87-3 CAPLUS
     Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-[(hexyloxy)methyl]-,
CN
     chloride (9CI) (CA INDEX NAME)
/ Structure 83 in filė .gra /
RN
     404965-88-4 CAPLUS
     Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-[(heptyloxy)methyl]-,
CN
     chloride (9CI) (CA INDEX NAME)
/ Structure 84 in file .gra /
     404965-89-5 CAPLUS
RN
     Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-[(octyloxy)methyl]-,
CN
     chloride (9CI) (CA INDEX NAME)
/ Structure 85 in file .gra /
RN
     404965-90-8 CAPLUS
     Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-[(nonyloxy)methyl]-,
CN
     chloride (9CI) (CA INDEX NAME)
```

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/ Structure 86 in file .gra /
     404965-91-9 CAPLUS
RN
     Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-[(decyloxy)methyl]-,
CN
     chloride (9CI) (CA INDEX NAME)
/ Structure 87 in file .gra /
     404965-92-0 CAPLUS
RN
     Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-[(undecyloxy)methyl]-,
CN
     chloride (9CI) (CA INDEX NAME)
/ Structure 88 in file .gra /
     404965-93-1 CAPLUS
RN
     Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-[(dodecyloxy)methyl]-,
CN
     chloride (9CI) (CA INDEX NAME)
/ Structure 89 in file .gra /
     404965-94-2 CAPLUS
RN
     Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-(propoxymethyl)-,
CN
     iodide (9CI) (CA INDEX NAME)
/ Structure 90 in file .gra /
    404965-96-4 CAPLUS
RN
    Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-(propoxymethyl)-,
CN
     (OC-6-11) -hexafluoroantimonate(1-) (9CI) (CA INDEX NAME)
    CM
         1
    CRN 404965-95-3
    CMF C16 H20 N5 O
/ Structure 91 in file .gra /
         2
    CM
     CRN 17111-95-4
     CMF F6 Sb
     CCI CCS
/ Structure 92 in file .gra /
     404965-98-6 CAPLUS
RN
    Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-(butoxymethyl)-,
CN
    perchlorate (9CI) (CA INDEX NAME)
     CM
          1
     CRN 404965-97-5
     CMF C17 H22 N5 O
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/ Structure 93 in file .gra /
     CM
         2
     CRN 14797-73-0
    CMF Cl O4
/ Structure 94 in file .gra /
    404965-99-7 CAPLUS
RN
    Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-(butoxymethyl)-,
CN
    nitrate (9CI) (CA INDEX NAME)
     CM
     CRN
         404965-97-5
     CMF
         C17 H22 N5 O
/ Structure 95 in file .gra /
    CM
         2
    CRN 14797-55-8
     CMF N O3
/ Structure 96 in file .gra /
    404966-00-3 CAPLUS
RN
    Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-(propoxymethyl)-,
CN
    hexafluorophosphate(1-) (9CI) (CA INDEX NAME)
    CM
         1
     CRN 404965-95-3
     CMF C16 H20 N5 O
/ Structure 97 in file .gra /
     CM
     CRN 16919-18-9
     CMF F6 P
     CCI CCS
/ Structure 98 in file .gra /
     404966-01-4 CAPLUS
RN
     Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-(propoxymethyl)-,
CN
     tetrafluoroborate(1-) (9CI) (CA INDEX NAME)
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10/717,958
     CM
         404965-95-3
     CRN
     CMF
         C16 H20 N5 O
/ Structure 99 in file .gra /
     CM
          2
         14874-70-5
     CRN
         B F4
     CMF
     CCI CCS
/ Structure 100 in file .gra /
RN
     404966-02-5 CAPLUS
     Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-(butoxymethyl)-,
CN
     iodide (9CI) (CA INDEX NAME)
/ Structure 101 in file .gra /
     A novel class of 3-substituted pyridinium salts have been
     synthesized in high yield by a convenient two-step procedure. A
     new synthetic pathway to 1-substituted benzimidazolium salts has been
     developed and the effects of the anionic component of the salts have been
     studied.
                                THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS
REFERENCE COUNT:
                          18
                                RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
     ANSWER 6 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN
                          1989:614902 CAPLUS
ACCESSION NUMBER:
DOCUMENT NUMBER:
                          111:214902
                         \alpha, \omega-Di(phosphonomethyl) and
TITLE:
                         \alpha, \omega-di (methylphosphinomethyl)
                         L-\alpha, \omega-diamino acids
                         Nachev, I.
AUTHOR(S):
                         Res. Cent. "Konstrukcionni Polymeri", Sofia, 1528,
CORPORATE SOURCE:
                         Bulq.
                          Izvestiya po Khimiya (1988), 21(4), 477-83
SOURCE:
                          CODEN: IZKHDX; ISSN: 0324-0401
                          Journal
DOCUMENT TYPE:
                         Bulgarian
LANGUAGE:
                         CASREACT 111:214902
OTHER SOURCE(S):
     123529-71-5P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation and reactions with Et phosphite or methylphosphonite)
     123529-71-5 CAPLUS
RN
     Acetamide, N-[(acetyloxy)methyl]-N-[1-[(acetyloxy)methyl]-2-oxo-3-
CN
    piperidinyl]-, (S)- (9CI) (CA INDEX NAME).
Absolute stereochemistry.
/ Structure 102 in file .gra /
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GI

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/ Structure 103 in file .gra /
     Treatment of the lactams of L-2,4-diaminobutanoic acid, L-ornithine, or
     L-lysine with HCHO in the presence 1,10-phenanthroline Co complex,
    followed by (CF3CO) 20 in AcOH, afforded acetoxymethylated derivs. I (n =
     1, 2, 3; R = AcOH). Condensation of the latter with P(OEt)3 or MeP(OEt)2
     gave phosphorus derivs. I [R = R1P(O)OEt, R1 = OEt, Me]. Hydrolysis of
     the P ester groups with phosphodiesterase I and alkaline hydrolysis of the
     lactam ring and the acetyl group afforded title amino acids
     HOPR1 (O) CH2NHCH (CO2) n+1NHCH2PR1 (O) OH.
    ANSWER 7 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN
                         1978:542494 CAPLUS
ACCESSION NUMBER:
DOCUMENT NUMBER:
                         89:142494
                         Aging of soman-inhibited acetylcholinesterase:
TITLE:
                         inhibitors and accelerators
                         Schoene, K.
AUTHOR(S):
                         Inst. Aerobiol., Fraunhofer-Ges., Schmallenberg-Grafschaft, Fed. Rep. Ger.
CORPORATE SOURCE:
                         Biochimica et Biophysica Acta (1978), 525(2), 468-71
SOURCE:
                         CODEN: BBACAQ; ISSN: 0006-3002
                         Journal
DOCUMENT TYPE:
                         English
LANGUAGE:
     61360-43-8 61368-95-4
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, with soman-inhibited acetylcholinesterase, aging in
        relation to)
     61360-43-8 CAPLUS
RN
     Pyridinium, 1,1'-[oxybis(methylene)]bis[3-[(aminocarbonyl)amino]-,
CN
     dichloride (9CI) (CA INDEX NAME)
/ Structure 104 in file .gra /
     61368-95-4 CAPLUS
RN
     Pyridinium, 1,1'-[oxybis(methylene)]bis[3-(acetylamino)-, dichloride (9CI)
CN
       (CA INDEX NAME)
/ Structure 105 in file .gra /
     The influence of 27 possible effectors, mostly bispyridinium salts, on the
     dealkylation (aging) of soman-inhibited acetylcholinesterase was examined at
     pH 7.6 and 25°. In the absence of effectors, the rate constant of
     the aging process was 4.0 + 10-2 min-1. At 2 mM, the
     strongest inhibitor reduced the rate to 0.8 + 10-2 min-1, whereas it
     was raised to 8.2 + 10-2 min-1 by the most potent accelerator.
     ANSWER 8 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN
                         1970:402338 CAPLUS
ACCESSION NUMBER:
                         73:2338
DOCUMENT NUMBER:
                         Relation between chemical structure and cholinesterase
TITLE:
                         reactivating effect in a number of new asymmetric
                         bis-quaternary pyridinium salts. I. Derivatives of
                         4-hydroxyiminomethylpyridine
                         Dirks, E.; Scherer, A.; Schmidt, Max; Zimmer, Gerhard
AUTHOR (S):
                         Battelle-Inst. e.V., Frankfurt/M., Fed. Rep. Ger.
CORPORATE SOURCE:
                         Arzneimittel-Forschung (1970), 20(1), 55-62
SOURCE:
```

CN

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CODEN: ARZNAD; ISSN: 0004-4172
DOCUMENT TYPE:
                         Journal
                         German
LANGUAGE:
     27844-72-0 31984-53-9
TT
     RL: BIOL (Biological study)
        (cholinesterase reactivation by)
     27844-72-0 CAPLUS
RN
     Pyridinium, 3-(dimethylamino)-1-[[[4-[(hydroxyimino)methyl]pyridinio]metho
     xy]methyl]-, dichloride (9CI) (CA INDEX NAME)
/ Structure 106 in file .gra /
     31984-53-9 CAPLUS
RN
     Pyridinium, 3-amino-4'-formyl-1,1'-(oxydimethylene)di-, dichloride, oxime
CN
           (CA INDEX NAME)
/ Structure 107 in file .gra /
     Two series of asymmetric bis(pyridinium) salts, characterized by a
AB
     methylene or O link joining the N atoms of the pyridine nuclei and having
     a p-aldoxime substituent on 1 of the pyridine nuclei were
     synthesized, including 1-[3-(3-dimethylamino-1-pyridinyl)propyl]-
     pyridine-4-aldoxime dibromide, 1-[3-(3-fluoro-1-pyridinyl),-2-
     oxapropyl]pyridine-4-aldoxime dichloride, 1-[3-(4-methoxy-1-
     pyridinyl)propyl]pyridine-4-aldoxime dibromide, and 1-[3-(4-tert-butyl-
     pyridinyl)-2-oxapropyl]pyridine-4-aldoxime dichloride. The ability of
     these compds. to reactivate acetylcholinesterase, previously inhibited by
     diisopropylfluorophosphate, as well as their inhibitory effect on
     untreated enzyme, depended on the radical added to the pyridine nuclei and
     on the nature of the bridge member. The size of the radical and its
     ability to dissociate into ions appear to be the essential factors, the
     electronic and phys. properties characterized by the Hammett
     \sigma\text{-consts.} and the Rf values being less important. The aldoxime
     radical had little effect on the activity of these compds., since it could
     be replaced by other radicals without affecting the results substantially.
     No significant relations between the increase in the hydrolysis rate of
     diisopropylfluorophosphate in the presence of bis(pyridinium) salts and
     their reactivating effect, or between the acute toxicity of the salts and
     their inhibitory effects on acetylcholine-esterase, were observed
     ANSWER 9 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN
                         1970:111249 CAPLUS
ACCESSION NUMBER:
                         72:111249
DOCUMENT NUMBER:
                         Relation between chemical structure and cholinesterase
TITLE:
                         reactivating effect in new asymmetric pyridinium
                        salts. II. Derivatives of 2-
                         hydroxyiminomethylpyridine
                         Dirks, E.; Scherer, A.; Schmidt, Max; Zimmer, Gerhard
AUTHOR (S):
                         Battelle-Inst. e. V., Frankfurt/M., Fed. Rep. Ger.
CORPORATE SOURCE:
                         Arzneimittel-Forschung (1970), 20(2), 197-200
SOURCE:
                         CODEN: ARZNAD; ISSN: 0004-4172
                         Journal
DOCUMENT TYPE:
                         German
LANGUAGE:
     27183-61-5P 27183-62-6P
     RL: SPN (Synthetic preparation); PREP (Preparation)
         (preparation of)
     27183-61-5 CAPLUS
RN
     Pyridinium, 3'-amino-2-formyl-1,1'-(oxydimethylene)di-, dichloride, oxime
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(CA INDEX NAME) (8CI)

/ Structure 108 in file .gra /

27183-62-6 CAPLUS
Pyridinium, 1-[[[3-(dimethylamino)pyridinio]methoxy]methyl]-2-CN [(hydroxyimino)methyl]-, dichloride (9CI) (CA INDEX NAME)

/ Structure 109 in file .gra /

For diagram(s), see printed CA Issue. GI

I (Q = CH2 or O; R = m- or p-NO2, MeSO2, F, Cl, Br, I, SMe, NH2, NMe2, AB tert-Bu, MeO, CH:NOH, CO2H, or CHN+Me3; X = Cl or Br) were prepd . by authors' (1970) methods. I with R in the m-position did not reactivate acetylcholinesterase (EC. 3.1.1.7) inhibited with diisopropyl fluorophosphate. I (R = p-tert-Bu) showed significant reactivating activity at 1.05 e 10-2 M. The reactivating activity of all I was lower than that of the corresponding p-aldoximes. I with large or polar R-substituents showed the lowest inhibiting activity on acetylcholinesterase. I (Q = O, R = m-substituent) showed the greatest inhibiting activity.

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